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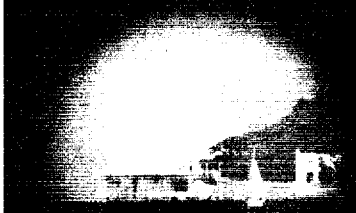

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Abstract

Using the effective field theory with a probability distribution technique that accounts for the self-spin correlation functions, the phase transitions in the semi-infinite anisotropic spin-$\frac{1}{2}$ Heisenberg ferromagnet on a simple cubic lattice are examined. For fixed values of the reduced exchange anisotropic parameter, the critical temperature of the system is studied as a function of the ratio R of the surface exchange couplings to the bulk ones. It was found that if $R \leq R_c$, the system orders at the bulk critical temperature T_c^B/J and if $R \geq R_c$, the system exhibits two successive transitions. The surface orders at the surface critical temperature T_c^S/J which is higher than T_c^B/J and as the temperature is lowered, in the presence of ordered surface, the bulk orders at T_c^B/J.

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1 Introduction

During the last decade, various types of approximations dealing with random Ising systems have appeared that employ an effective field theory to study the magnetic properties of such systems[1-12]. Recently one of the authors[13] of the present paper has developed a new version of the effective field theory which extends the approximation methods[11-12] to random Ising systems in which randomness can be described by discrete random variables and the geometry of the lattice can be easily taken into account. This method is based on the determination of the probability distribution of the discrete variables which takes into account exactly of the self-site correlations. This approach has been applied successfully to various physical problems such as diluted Ising systems, transverse Ising systems and thin films. This method can be developed within the framework of a n-site cluster approximation, although for mathematical simplicity and numerical tractability, most studies have adopted a single-site approximation. This approach of considering one-site cluster approximation does not apply to quantum spin systems.

On one hand to treat approximately quantum spin systems, Mielnicki et al.[14] and Idogaki et al.[15] introduced the application of the two-site cluster approximation to the diluted quantum anisotropic spin-$\frac{1}{2}$ Heisenberg system and interesting results were obtained. In this two-site approximation the Heisenberg ferromagnet is only described by a two-particle cluster containing two Heisenberg spins surrounded by Ising spins, that is all the quantum spins surrounding the two-particle cluster are substituted by Ising spins and the exchange coupling between nearest neighbor spins will be taken into account.

On the other hand the problem of surface magnetism of the Ising system is very interesting[16-24]. When the ratio of the surface exchange interactions to the bulk ones $R = J_s/J$ is larger than a critical value R_c, the system becomes ordered on the surface before it is ordered in the bulk, and the critical temperature of the surface T_c^S/J is higher than that of the bulk T_c^B/J and if R is less than R_c, the system orders at the bulk critical temperature T_c^B/J. The phase transitions in the infinite bulk anisotropic Heisenberg ferromagnetic systems were investigated[25-26]. The ferromagnetism which is absent in two dimensional isotropic Heisenberg model[27] can be restored by an arbitrary small anisotropy[28]. Therefore, it is very interesting to investigate the critical properties of the semi-infinite anisotropic spin-$\frac{1}{2}$ Heisenberg ferromagnet. But, to our knowledge, apart the study of the tricritical behavior by Wu and Li[29] in the semi-infinite anisotropic Heisenberg ferromagnet due to the presence of a random longitudinal field at the surface there is no studies of the phase transitions in such a system.

The purpose of this paper is to investigate the critical behavior of the anisotropic ferromagnet spin-$\frac{1}{2}$ Heisenberg system by extending the effective field theory with the probability distribution technique established for the single-site cluster approximation to the two-site cluster approximation in order to study approximately the phase transitions

in the semi-infinite anisotropic spin-$\frac{1}{2}$ Heisenberg ferromagnet on a simple cubic lattice. In section 2, we describe briefly the model and generalize the single-site cluster approximation to two-site cluster approximation within the framework of the effective field theory with a probability distribution technique. The results of the phase diagrams of the semi-infinite system are presented in section 3. The last section 4 is devoted to a brief conclusion.

2 The model and the results

We consider the anisotropic ferromagnet spin-$\frac{1}{2}$ Heisenberg model on a simple cubic lattice which is described by the hamiltonian

$$H = -J \sum_{(i,j)} [\sigma_{iz}\sigma_{jz} + \alpha(\sigma_{ix}\sigma_{jx} + \sigma_{iz}\sigma_{jz})], \tag{1}$$

where J is the ferromagnetic exchange coupling ($J > 0$), α is the exchange anisotropic parameter ($0 \leq \alpha \leq 1$) and σ_{ix}, σ_{iy} and σ_{iz} denote the Pauli matrices which are the components of the quantum spin $\vec{\sigma_i}$ of magnitude $\sigma = \frac{1}{2}$ at site i, and the summation runs over all pairs of nearest neighbors.

In its simplest form the effective field theory is based on a two-site cluster theory in which attention is focused on a cluster comprising just two selected Heisenberg spins, labelled 1 and 2, and the neighboring Ising spins with which it directly interacts.

To this end the hamiltonian is approximated by $H = H_{12} + H_1 + H_2$, where H_{12} is that part of the hamiltonian containing the spins 1 and 2 namely:

$$H_{12} = -J[\sigma_{1z}\sigma_{2z} + \alpha(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y})] \tag{2}$$

and H_1 (H_2) is the Ising Hamiltonian type, namely

$$H_1 = -J(\sum_{i_1 \neq 1}^{N-1} \sigma_{i_1 z})\sigma_{1z} \tag{3}$$

$$H_2 = -J(\sum_{i_2 \neq 2}^{N-1} \sigma_{i_2 z})\sigma_{2z}. \tag{4}$$

The starting point of the two-site cluster approximation is a set of formal identities of the type

$$< \sigma_z >= \frac{1}{2} < \sigma_{1z} + \sigma_{2z} >= \frac{1}{2} < \frac{trace_{1,2}[(\sigma_{1z} + \sigma_{2z}) \exp(-\beta(H_{12} + H_1 + H_2))]}{trace_{1,2}[\exp(-\beta(H_{12} + H_1 + H_2))]} > . \tag{5}$$

Evaluation of the $trace_{1,2}$ on the right-hand side of this equation leaves one with a transcendental function whose argument contains operators belonging to spins with which the central spins $\vec{\sigma_1}$ and $\vec{\sigma_2}$ interact. For the system under consideration, in the case when

the exchange interactions are between nearest neighbor sites only, one finds (for a fixed spatial configuration of the spins)

$$< \sigma_z >=< F(\sum_{i_1 \neq 1}^{N-1} \sigma_{i_1 z}, \sum_{i_2 \neq 2}^{N-1} \sigma_{i_2 z}) >, \tag{6}$$

where in particular

$$F(x_1, x_2) = \frac{1}{2} \frac{sinh(\frac{1}{2}\beta J(x_1 + x_2))}{cosh(\frac{1}{2}\beta J(x_1 + x_2)) + exp(-\frac{1}{2}\beta J) cosh[\frac{1}{2}\beta J \sqrt{(x_1 - x_2)^2 + a^2}]}. \tag{7}$$

The sums in Eq. (6) are over the $N-1$ nearest neighbors of the site $\vec{\sigma_1}$ and $(\vec{\sigma_2})$, N being the nearest neighbor coordination number of the lattice ($N = 6$ for the case of a simple cubic lattice which is considered here). In a mean field approximation one would simply replace these spin operators by their thermal values. However, it is at this point that a substantial improvement to the theory is made by noting that the z components of the spin operators have a finite set of base states, so that the average over the function F can be expressed as an average over a finite polynomial of the z-components σ_z of the spin operators belonging to the neighboring spins. This procedure can be effected by the combinatorial method and correctly accounts for the single site kinematic relations. Up to this point the right-hand side of Eq. (6) will contain multiple spin correlation functions. Usually, at this stage a Zernike type decoupling of the multiple spin correlation functions is made that neglects the correlation between quantities pertaining to different sites.

The above thermal averages were for a fixed spatial configuration. In the next step, when computing the average over configurations, the correlations between different sites will be neglected. This is the approach we adopt here using the effective field theory with the probability distribution technique[13]. In this approach the z-components σ_z of the spin $\vec{\sigma}$ are random variables which obey the following probability distribution law

$$P(\sigma_{iz}) = \frac{1}{2}[(1 - 2m_z)\delta(\sigma_{iz} + \frac{1}{2}) + (1 + 2m_z)\delta(\sigma_{iz} - \frac{1}{2})] \tag{8}$$

with

$$m_z =< \sigma_{iz} > . \tag{9}$$

Eqs. (6), (8) and (9) yield the following expression for the longitudinal magnetization

$$m_z = 2^{-2(N-1)} \sum_{\mu=0}^{N-1} \sum_{\nu=0}^{N-1} C_\mu^{(N-1)-\mu} C_\nu^{(N-1)-\nu} (1 - 2m_z)^{\mu+\nu} (1 + 2m_z)^{2(N-1)-(\mu+\nu)}$$
$$F[\frac{1}{2}((N-1) - 2\mu), \frac{1}{2}((N-1) - 2\nu)]. \tag{10}$$

We have thus obtained the self consistent equation Eq. (10) for the longitudinal magnetization m_z, that can be solved directly by numerical iteration. No further algebraic

manipulation is necessary. This is the advantage of introducing the probability distribution technique.

3 The phase diagrams

Let us begin with the evaluation of the bulk critical temperature versus the reduced exchange anisotropic parameter. The Curie temperature T_c^B/J is determined as the lowest temperature at which Eq. (10) has a non trivial solution $m_z \neq 0$. In other words, when Eq. (10) is expanded into power series of m_z, the coefficient of the linear term of m_z on the right-hand side is equal to unity at $T/J = T_c^B/J$. Thus the equation for T_c^B/J becomes

$$a_1 = 1 \tag{11}$$

where

$$a_1 = 2^{-2(N-1)} \sum_{\mu=0}^{N-1} \sum_{\nu=0}^{N-1} \sum_{i=0}^{\mu+\nu} \sum_{j=0}^{2(N-1)-(\mu+\nu)} C_\mu^{(N-1)-\mu} C_\nu^{(N-1)-\nu} C_i^{\mu+\nu} C_j^{2(N-1)-(\mu+\nu)}$$
$$(-1)^i 2^{i+j} \delta_{i+j,1} F[\frac{1}{2}((N-1)-2\mu), \frac{1}{2}((N-1)-2\nu)]. \tag{12}$$

The dependence of the bulk critical temperature on the reduced exchange anisotropic parameter α is shown in Fig. 1. As expected, the bulk critical temperature T_c^B/J decreases from its Ising value $\frac{T_c^B}{J}(\alpha = 0) = 1.2598$ with the increase of α to reach its lowest value which is the Heisenberg value at $\alpha = 1$ ($\frac{T_c^B}{J}(\alpha = 1) = 1.2228$). Our results are in agreement with those of Idogaki et al.[15] and Wu et al.[29]. Because $\vec{\sigma}^2 = \frac{1}{4}$, our numerical values are $\frac{1}{4}$ their values.

To study the semi-infinite system, we assume that the exchange coupling between the z-components of $\vec{\sigma}$ in Eq. (1) is J_s if both spins belong to the surface and J otherwise. For simplicity, we assume that the reduced exchange anisotropic parameter is the same both in the surface and in the bulk.

To study the critical properties of this system, we follow Binder and Hohenberg[30]. We suppose that the system is a film formed of layers and we allow for the site magnetizations to take different values in each atomic layer parallel to the surface of the film, and label them in accordance with the layer number in which they are situated. Near the critical temperature, each layer magnetization is small. By expanding the analogous of Eq. (10) for this system and keeping only linear terms in the magnetization, we get the following set of equations for the layer longitudinal magnetizations,

$$m_{1z} = a_{11} m_{1z} + a_{12} m_{2z} \tag{13}$$

$$m_{2z} = a_{21} m_{1z} + a_{22} m_{2z} + a_{23} m_{3z} \tag{14}$$

.....

$$m_{nz} = a_{n-1,n} m_{n-1,z} + a_{nn} m_{nz} + a_{n.n+1} m_{n+1,z} \tag{15}$$

where

$$a_{11} = 2^{-2(N-3-N_0)} \sum_{\mu_1=0}^{N-3} \sum_{\mu_2=0}^{N-3} \sum_{\nu_1=0}^{N_0} \sum_{\nu_2=0}^{N_0} \sum_{i=0}^{\mu_1+\mu_2} \sum_{j=0}^{2(N-3)-(\mu_1+\mu_2)} C_{\mu_1}^{N-3} C_{\mu_2}^{N-3} C_{\nu_1}^{N_0} C_{\nu_2}^{N_0}$$
$$C_i^{\mu_1+\mu_2} C_j^{2(N-3)-(\mu_1+\mu_2)} (-1)^i 2^{i+j} \delta_{i+j,1} F(x_{11}, x_{12}) \tag{16}$$

$$a_{12} = 2^{-2(N-3-N_0)} \sum_{\mu_1=0}^{N-3} \sum_{\mu_2=0}^{N-3} \sum_{\nu_1=0}^{N_0} \sum_{\nu_2=0}^{N_0} \sum_{i=0}^{\nu_1+\nu_2} \sum_{j=0}^{2N_0-(\nu_1+\nu_2)} C_{\mu_1}^{N-3} C_{\mu_2}^{N-3} C_{\nu_1}^{N_0} C_{\nu_2}^{N_0}$$
$$C_i^{\nu_1+\nu_2} C_j^{2N_0-(\nu_1+\nu_2)} (-1)^i 2^{i+j} \delta_{i+j,1} F(x_{11}, x_{12}) \tag{17}$$

and for $n \geq 2$ we have

$$a_{n,n-1} = 2^{-2(N-3-2N_0)} \sum_{\mu_1=0}^{N-3} \sum_{\mu_2=0}^{N-3} \sum_{\nu_1=0}^{N_0} \sum_{\nu_2=0}^{N_0} \sum_{\rho_1=0}^{N_0} \sum_{\rho_2=0}^{N_0} \sum_{i=0}^{\rho_1+\rho_2} \sum_{j=0}^{2N_0-(\rho_1+\rho_2)} C_{\mu_1}^{N-3} C_{\mu_2}^{N-3}$$
$$C_{\nu_1}^{N_0} C_{\nu_2}^{N_0} C_{\rho_1}^{N_0} C_{\rho_2}^{N_0} C_i^{\rho_1+\rho_2} C_j^{2N_0-(\rho_1+\rho_2)} (-1)^i 2^{i+j} \delta_{i+j,1} F(x_{n1}, x_{n2}) \tag{18}$$

$$a_{n,n} = 2^{-2(N-3-2N_0)} \sum_{\mu_1=0}^{N-3} \sum_{\mu_2=0}^{N-3} \sum_{\nu_1=0}^{N_0} \sum_{\nu_2=0}^{N_0} \sum_{\rho_1=0}^{N_0} \sum_{\rho_2=0}^{N_0} \sum_{i=0}^{\mu_1+\mu_2} \sum_{j=0}^{2(N-3)-(\mu_1+\mu_2)} C_{\mu_1}^{N-3} C_{\mu_2}^{N-3}$$
$$C_{\nu_1}^{N_0} C_{\nu_2}^{N_0} C_{\rho_1}^{N_0} C_{\rho_2}^{N_0} C_i^{\mu_1+\mu_2} C_j^{2(N-3)-(\mu_1+\mu_2)} (-1)^i 2^{i+j} \delta_{i+j,1} F(x_{n1}, x_{n2}) \tag{19}$$

$$a_{n,n+1} = 2^{-2(N-3-2N_0)} \sum_{\mu_1=0}^{N-3} \sum_{\mu_2=0}^{N-3} \sum_{\nu_1=0}^{N_0} \sum_{\nu_2=0}^{N_0} \sum_{\rho_1=0}^{N_0} \sum_{\rho_2=0}^{N_0} \sum_{i=0}^{\nu_1+\nu_2} \sum_{j=0}^{2N_0-(\nu_1+\nu_2)} C_{\mu_1}^{N-3} C_{\mu_2}^{N-3}$$
$$C_{\nu_1}^{N_0} C_{\nu_2}^{N_0} C_{\rho_1}^{N_0} C_{\rho_2}^{N_0} C_i^{\nu_1+\nu_2} C_j^{2N_0-(\nu_1+\nu_2)} (-1)^i 2^{i+j} \delta_{i+j,1} F(x_{n1}, x_{n2}), \tag{20}$$

with

$$x_{11} = \frac{1}{2}[R((N-3) - 2\mu_1) + (N_0 - 2\nu_1)] \tag{21}$$

$$x_{12} = \frac{1}{2}[R((N-3) - 2\mu_2) + (N_0 - 2\nu_2)] \tag{22}$$

.....

$$x_{n1} = \frac{1}{2}[(N-3) - 2\mu_1) + (N_0 - 2\nu_1) + (N_0 - 2\rho_1)] \tag{23}$$

$$x_{n2} = \frac{1}{2}[(N-3) - 2\mu_1) + (N_0 - 2\nu_1) + (N_0 - 2\rho_1)]. \tag{24}$$

According to Binder and Hohenberg[30], let us assume that $m_{n+1,z} = \gamma m_{nz}$ for $n \geq 3$, e. g. the layer longitudinal magnetization m_{nz} of each layer with n larger than 2 decreases exponentially into the bulk. Eqs. (13) and (14) then yield the following secular equation

$$M_s \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} a_{11} - 1 & a_{12} \\ a_{21} & a_{22} + \gamma a_{23} - 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = 0, \tag{25}$$

where the parameter γ is given by, using Eq. (15)

$$\gamma = \frac{(1 - a_{nn}) - \sqrt{(1 - a_{nn})^2 - 4a_{n,n-1}a_{n,n+1}}}{2a_{n,n+1}}. \tag{26}$$

Thus the surface critical temperature T_c^S/J can be derived from the condition $det\ M_s = 0$, namely

$$(a_{11} - 1)(a_{22} + \gamma a_{23} - 1) - a_{12}a_{21} = 0. \tag{27}$$

We are now in a position to examine the physical properties for the surface and the bulk of the semi-infinite system numerically. Here it is worth nothing that in our treatment the bulk transition temperature T_c^B/J can be determined by putting $m_{nz} = m_{n-1,z} = m_{n+1,z} = m_z$ into Eq. (15), i. e.

$$1 = a_{n,n-1} + a_{n,n} + a_{n,n+1} \tag{28}$$

which is equivalent to Eq. (11).

The variation of the critical temperature of the semi-infinite anisotropic Heisenberg system T_c/J as a function of the ratio of the surface exchange interactions to the bulk ones $R = J_s/J$ for several values of the reduced exchange anisotropic parameter α is shown in Fig. 2. The solid, dashed and dotted curves correspond respectively to $\alpha = 0, 0.5$ and 1. All the curves are very similar, in the sense that for any value of α, $(0 \leq \alpha \leq 1$, the system orders at the bulk critical temperature T_c^B/J if $R \leq R_c = R_c(\alpha)$ and if $R \geq R_c$, the system becomes ordered at the surface before it is ordered in the bulk and the critical temperature of the surface T_c^S/J is higher than T_c^B/J. We see also that the critical temperatures of the semi-infinite system decease with the increase of the reduced exchange anisotropic parameter α as it does for the infinite bulk system.

4 Conclusion

We have investigated the influence of the reduced exchange anisotropic parameter α on the critical temperatures of the semi-infinite anisotropic Heisenberg model on a simple cubic lattice. By assuming α to be the same on the surface and in the bulk and depending of the ratio of the surface exchange interactions to the bulk ones $R = J_s/J$, we show that this model orders at the bulk critical temperature if R is less than a critical value R_c which depends on α and if R is larger than R_c, the system becomes ordered on the surface at the surface critical temperature T_c^S/J greater than T_c^B/J before it is ordered in the bulk.

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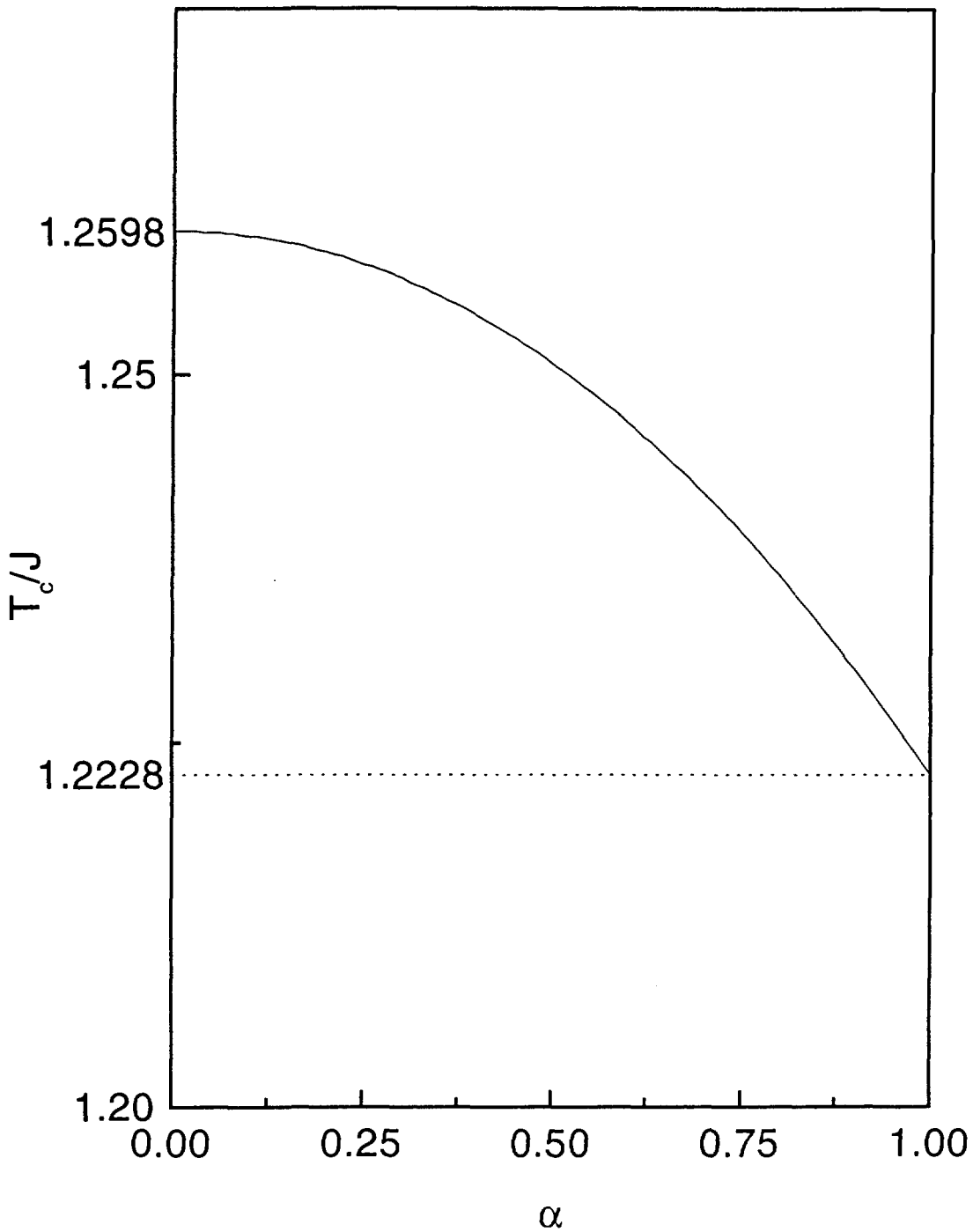

Fig. 1: The dependence of the bulk critical temperature T_c^B/J on the reduced exchange anisotropic parameter α for the anisotropic Heisenberg model on a simple cubic lattice.

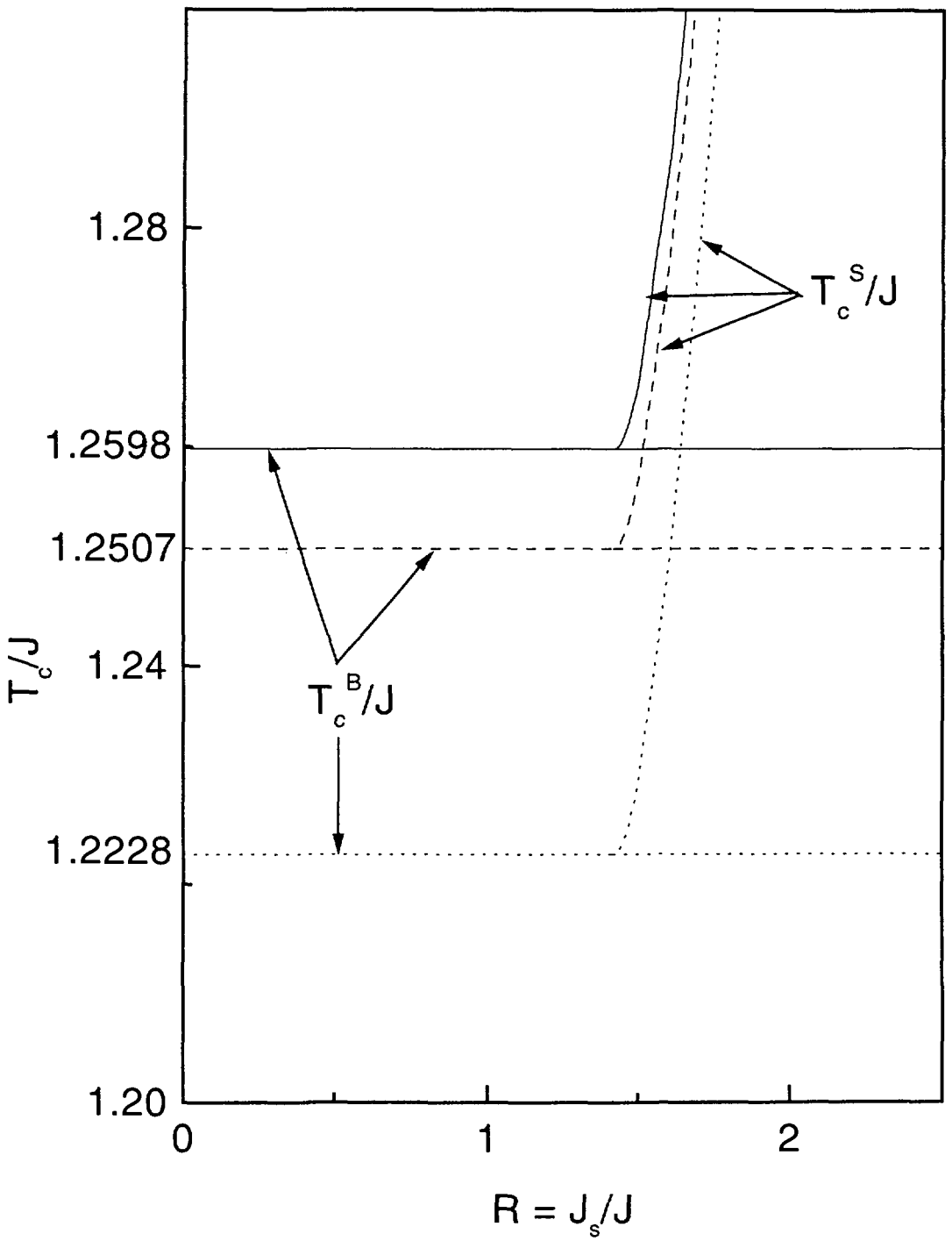

Fig. 2: The dependence of critical temperature T_c/J on the ratio of the surface exchange interactions to the bulk ones $R = J_s/J$ for the anisotropic Heisenberg model on a simple cubic lattice for several values of α.